

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.44e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.89e-01

Confidence level: 5.28e-01

Nearest Neighbors from the Training Set

Image not found

2-PTERIDINAMINE

Measured: 5.04e-03

Predicted: 1.72e-02